Chem 312: Physical Chemistry II
Spring 2005

Prof. Tom Varberg (OR317, 696–6468)
Class meets MWF 8:30 – 9:30 in OR301

Date	Day	Ch	Subject	Laboratory (Thursdays 1:00)
1/24	M	23	Diffraction methods	
26	W	23		Crystal models
28	F	23		
31	M	11	Introduction to quantum theory	
2/2	W		*Introduction of XRD lab*	NaCl/KCl phase diagram/XRD
4	F	11		(joint with Petrology class)
7	M	11		
9	W	12	Applications of quantum theory	Spectrum of β-carotene
11	F	12		
14	M		*Oral presentations of XRD lab: 8:00 AM*	
16	W	12		Computational chemistry I
18	F	12		
21	M	13	Atomic structure and spectroscopy	
23	W	13		**Exam 1 (during lab Thur 2/24)**
25	F	13		
28	M	14	Molecular structure	
3/2	W	14		Hückel calculations I
4	F	14		
7	M	14		
9	W	14	Computational chemistry	Computational chemistry II
11	F	14		
14	M	15	Symmetry	
16	W	15		Hückel calculations II
18	F	15		
21	M			
23	W		**Spring Break**	**Week!**
25	F			
28	M	15		
30	W	16	Rotational and vibrational spectroscopy	**Exam 2 (during lab Thur 3/31)**
4/1	F	16		
4	M	16		
6	W	16		Rovibrational spectrum of HCl
8	F	16		
11	M	17	Electronic spectroscopy	
13	W	17		Electronic spectrum of iodine
15	F	17		
18	M	17	Lasers	
20	W	19	Statistical thermodynamics	Scanning tunneling microscopy
22	F	19		
25	M	19		
27	W	20	Statistical thermodynamics	**Exam 3 (during lab Thur 4/28)**
29	F	20		
5/2	M	20		

Text: Peter Atkins and Julio de Paula, *Physical Chemistry*, 7th Ed., Freeman, New York, 2002.

Point distribution: The breakdown of the grading will be as follows.

300	Three exams (3 × 100)
150	Final exam
100	Problem sets
150	Laboratory
700	Total points

Final exam: The final examination for this class is scheduled for 8:00 to 10:00 am on Monday, May 9. This is the last scheduled day of finals; please make note of the date on your calendar now. The exam given will be an American Chemical Society Standardized Exam for Physical Chemistry.

Grades: The following grading scale will be applied in determining final grades for the course. While I expect to follow this scale quite closely, I reserve the right to lower the boundaries, but under no circumstance will I raise them. You should keep in mind that students in the past score significantly higher on the problem sets and labs than they do on the semester exams and the final. The boundaries shown are for the integer part of your final percentage (thus, a score of 85.9% is a B+).

Final grade	Final score
A	89–100%
A–	86–88
B+	83–85
B	79–82
B–	76–78
C+	73–75
C	66–72
C–	62–65
D+	58–61
D	54–57
D–	50–53
NC	< 50

Ombudsperson: Brinton Seashore–Ludlow (bseashorelud@macalester.edu) has agreed to serve as an ombudsperson for this class. If you have any concerns about the course that you would like to have addressed anonymously, you may direct them to her, and she can then speak to me about them.

Office Hours: M 3:30 – 4:30; WF 2:20 – 3:20

Problem sets: The following problem sets will be collected and graded during the course of the semester by the grader assigned to this class. A late penalty of 10% per weekday will be assessed for problems turned in after the due date, and *in no case are they accepted following the exam that covers that chapter*. Some of the problems assigned and/or their due dates may change as we progress through the syllabus, but announcements will be made in class and/or emailed to you to alert you to any such changes.

Weekly problem set assignments:

Due date	Chapter	Assigned **E**xercises and **P**roblems
M 1/31	23	**E** 7b, 8b, 13b; **P** 2, 4 (Note: to obtain the correct answer, assume the distance shown in the figure is 4.5 mm, not 1 cm. This problem must be done using a spreadsheet), 26, 29
W 2/9	11	**E** 11b, 13b, 15b, 18b, 19b; **P** 4, 8, 10, 14(b), 15, 16, 17, 20, 21(b)
M 2/21	12	**E** 9b, 12b, 17a, 17b, 18b; **P** 4 (use the exact masses found in the Table on pg. 1074), 12, 19(a,b), 20 [Note corrected form of Eqn. 12.62 shown below and on UIC.]
M 2/28	13	**E** 6b (2 of the 3 extrema can be found by differentiation), 11b, 12b, 15b, 17b, 18b, 19b, 22b, 23b; **P** 2, 5, 11, 12
M 3/14	14	**E** 5b, 6b, 7b, 8b, 11b (assume $S_{AB} = 0$); **P** 2, 3, 8, 9 (these four problems must be done on a spreadsheet; plot the curves for 8 and 9 on one graph) Together with a partner, generate a Walsh diagram of your favorite triatomic molecule. Walsh diagrams will be described in class.
Tu 3/29 noon	15	*Note:* You will need the D_{6h} and D_{4h} character tables to complete this assignment; these will be handed out in class. **E** 5b, 7b, 8b, 13b, 16a, 17a; **P** 2, 8, 20 (D_{4h})
M 4/11	16	*Note:* For all problems in this chapter, you need to use the exact isotopic masses given in the table on very last page of the textbook. **E** 8b, 11b, 22b, 27b, 29a (This should read "Show that the displacements span…"; also please identify the IR and Raman active modes); **P** 4, 11 (the transition energies listed are in MHz, not m^{-1}), 16 (must be done using a spreadsheet), 19 (use MacSpartan)
W 4/20	17	**E** 11a; **P** 1, 11, 14, 25
W 4/27	19	TBA

Typographical errors: Please note that in the C_{4v} character table (p. 1108), the character of A_2 under the $2\sigma_d$ operation should read –1 (not 1). Also, Eq. (12.62) on p. 349 should read as follows: $\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Lambda^2$.